BETHE ANSATZ FOR THE OPEN XXZ CHAIN FROM FUNCTIONAL RELATIONS AT ROOTS OF UNITY

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We briefly review Bethe Ansatz solutions of the integrable open spin- $\frac{1}{2}$ XXZ quantum spin chain derived from functional relations obeyed by the transfer matrix at roots of unity.

1. Introduction

A long standing problem has been to solve the open spin- $\frac{1}{2}$ XXZ quantum spin chain with general integrable boundary terms, defined by the Hamiltonian 1,2

$$\mathcal{H} = \frac{1}{2} \left\{ \sum_{n=1}^{N-1} \left(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \operatorname{ch} \eta \ \sigma_n^z \sigma_{n+1}^z \right) + \operatorname{sh} \eta \left[\operatorname{cth} \alpha_- \operatorname{th} \beta_- \sigma_1^z + \operatorname{csch} \alpha_- \operatorname{sech} \beta_- \left(\operatorname{ch} \theta_- \sigma_1^x + i \operatorname{sh} \theta_- \sigma_1^y \right) - \operatorname{cth} \alpha_+ \operatorname{th} \beta_+ \sigma_N^z + \operatorname{csch} \alpha_+ \operatorname{sech} \beta_+ \left(\operatorname{ch} \theta_+ \sigma_N^x + i \operatorname{sh} \theta_+ \sigma_N^y \right) \right] \right\},$$

$$(1)$$

where σ^x , σ^y , σ^z are the standard Pauli matrices, η is the bulk anisotropy parameter, α_{\pm} , β_{\pm} , θ_{\pm} are arbitrary boundary parameters, and N is the number of spins. Determining the energy eigenvalues in terms of solutions of a system of Bethe Ansatz equations is a fundamental problem, which has important applications in integrable quantum field theory as well as condensed matter physics and statistical mechanics ³, and perhaps also string theory. (For an introduction to Bethe Ansatz, see e.g. Refs. 4, 5, 6.)

The basic difficulty in solving (1) is that, in contrast to the special case of diagonal boundary terms (i.e., α_{\pm} or $\beta_{\pm} \to \pm \infty$, in which case \mathcal{H} has

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a U(1) symmetry) which was solved long ago ^{7,8,9}, a simple pseudovacuum state does *not* exist. For instance, the state with all spins up is not an eigenstate of the Hamiltonian. Hence, many of the techniques which have been developed to solve integrable models cannot be applied.

We observed some time ago 10,11 that, for bulk anisotropy parameter values

$$\eta = \frac{i\pi}{p+1}, \qquad p = 1, 2, \dots$$
(2)

(hence $q \equiv e^{\eta}$ is a root of unity, satisfying $q^{p+1} = -1$) and arbitrary values of the boundary parameters, the model's transfer matrix t(u) (see Sec. 2) obeys a functional relation of order p+1. For example, for the case p=2, the functional relation is

$$t(u)t(u+\eta)t(u+2\eta) - \delta(u-\eta)t(u+\eta) - \delta(u)t(u+2\eta) - \delta(u+\eta)t(u) = f(u),$$
(3)

where $\delta(u)$ and f(u) are known scalar functions which depend on the boundary parameters. (Expressions for these functions in terms of the boundary parameters in (1) are given in Ref. 18.) Similar results had been known earlier for closed spin chains.^{12,13,14}

By exploiting these functional relations, we have obtained Bethe Ansatz solutions of the model for various special cases of the bulk and boundary parameters:

(i) [Refs. 15, 16, 17] The bulk anisotropy parameter has values (2); and the boundary parameters satisfy the constraint

$$\alpha_{-} + \beta_{-} + \alpha_{+} + \beta_{+} = \pm (\theta_{-} - \theta_{+}) + \eta k,$$
 (4)

where $k \in [-(N+1), N+1]$ is even (odd) if N is odd (even), respectively.

- (ii) [Ref. 18] The bulk anisotropy parameter has values (2) with p even; and either
 - (a) at most one of the boundary parameters is nonzero, or
 - (b) any two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are arbitrary, the remaining boundary parameters from this set are either η or $i\pi/2$, and $\theta_- = \theta_+$.
- (iii) [Ref. 19] The bulk anisotropy parameter has values (2) with p odd; at most two of the boundary parameters $\{\alpha_{-}, \alpha_{+}, \beta_{-}, \beta_{+}\}$ are nonzero, and $\theta_{-} = \theta_{+}$.

All of these cases have the property that the quantity $\Delta(u)$, defined by

$$\Delta(u) = f(u)^2 - 4 \prod_{j=0}^{p} \delta(u + j\eta),$$
 (5)

is a perfect square.

Solutions for generic values of the bulk anisotropy parameter and for boundary parameters obeying a constraint similar to (4) have been discussed in Refs. 20, 21, 22.

Here we briefly review our results for the cases (i) - (iii).

2. Transfer matrix

The transfer matrix t(u) of the open XXZ chain with general integrable boundary terms, which satisfies the fundamental commutativity property [t(u), t(v)] = 0, is given by ⁹

$$t(u) = \operatorname{tr}_0 K_0^+(u) \ T_0(u) \ K_0^-(u) \ \hat{T}_0(u) , \qquad (6)$$

where $T_0(u)$ and $\hat{T}_0(u)$ are the monodromy matrices

$$T_0(u) = R_{0N}(u) \cdots R_{01}(u), \qquad \hat{T}_0(u) = R_{01}(u) \cdots R_{0N}(u), \qquad (7)$$

and tr_0 denotes trace over the "auxiliary space" 0. The R matrix is given by

$$R(u) = \begin{pmatrix} \sinh(u+\eta) & 0 & 0 & 0\\ 0 & \sin u & \sin \eta & 0\\ 0 & \sin \eta & \sin u & 0\\ 0 & 0 & 0 & \sin(u+\eta) \end{pmatrix}, \tag{8}$$

where η is the bulk anisotropy parameter; and $K^{\mp}(u)$ are 2×2 matrices whose components are given by 1,2

$$\begin{split} K_{11}^{-}(u) &= 2 \left(\operatorname{sh} \alpha_{-} \operatorname{ch} \beta_{-} \operatorname{ch} u + \operatorname{ch} \alpha_{-} \operatorname{sh} \beta_{-} \operatorname{sh} u \right) \\ K_{22}^{-}(u) &= 2 \left(\operatorname{sh} \alpha_{-} \operatorname{ch} \beta_{-} \operatorname{ch} u - \operatorname{ch} \alpha_{-} \operatorname{sh} \beta_{-} \operatorname{sh} u \right) \\ K_{12}^{-}(u) &= e^{\theta_{-}} \operatorname{sh} 2u \,, \qquad K_{21}^{-}(u) = e^{-\theta_{-}} \operatorname{sh} 2u \,, \end{split} \tag{9}$$

and

$$K^{+}(u) = K^{-}(-u - \eta) \bigg|_{\alpha_{-} \to -\alpha_{+}, \beta_{-} \to -\beta_{+}, \theta_{-} \to \theta_{+}},$$
(10)

where α_{\mp} , β_{\mp} , θ_{\mp} are the boundary parameters. The Hamiltonian (1) is proportional to t'(0) plus a constant.

The transfer matrix also has $i\pi$ periodicity

$$t(u+i\pi) = t(u), \tag{11}$$

crossing symmetry

$$t(-u - \eta) = t(u), \tag{12}$$

and the asymptotic behavior

$$t(u) \sim -\operatorname{ch}(\theta_{-} - \theta_{+}) \frac{e^{u(2N+4)+\eta(N+2)}}{2^{2N+1}} \mathbb{I} + \dots$$
 for $u \to \infty$. (13)

3. Case (i)

Our main objective is to determine the eigenvalues $\Lambda(u)$ of the transfer matrix t(u) (6), from which the energy eigenvalues can readily be computed. The functional relations for the transfer matrix (e.g., (3)) evidently imply corresponding relations for $\Lambda(u)$. Following Ref. 23, we observe that the latter relations can be written as

$$\det \mathcal{M}(u) = 0, \tag{14}$$

where $\mathcal{M}(u)$ is the $(p+1) \times (p+1)$ matrix

$$\mathcal{M}(u) = \begin{pmatrix} \Lambda(u) & -\frac{\delta(u)}{h(u+\eta)} & 0 & \dots & 0 & -h(u) \\ -h(u+\eta) & \Lambda(u+\eta) & -\frac{\delta(u+\eta)}{h(u+2\eta)} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\frac{\delta(u-\eta)}{h(u)} & 0 & 0 & \dots & -h(u+p\eta) & \Lambda(u+p\eta) \end{pmatrix}$$
(15)

if there exists an $i\pi$ -periodic function h(u) such that

$$f(u) = \prod_{j=0}^{p} h(u+j\eta) + \prod_{j=0}^{p} \frac{\delta(u+j\eta)}{h(u+j\eta)}.$$
 (16)

To solve for h(u), we set $z(u) \equiv \prod_{j=0}^{p} h(u+j\eta)$, and observe that (16) implies that z(u) satisfies a quadratic equation

$$z(u)^{2} - z(u)f(u) + \prod_{j=0}^{p} \delta(u+j\eta) = 0,$$
(17)

whose solution is evidently given by

$$z(u) = \frac{1}{2} \left(f(u) \pm \sqrt{\Delta(u)} \right), \tag{18}$$

where $\Delta(u)$ is defined in (5). If the boundary parameters satisfy the constraint (4), then $\Delta(u)$ is a perfect square, and two solutions of (16) are

$$h^{(\pm)}(u) = -4 \operatorname{sh}^{2N}(u+\eta) \frac{\operatorname{sh}(2u+2\eta)}{\operatorname{sh}(2u+\eta)} \times \operatorname{sh}(u \pm \alpha_{-}) \operatorname{ch}(u \pm \beta_{-}) \operatorname{sh}(u \pm \alpha_{+}) \operatorname{ch}(u \pm \beta_{+}).$$
 (19)

Let us now label the corresponding matrices (15) by $\mathcal{M}^{(\pm)}(u)$.

The condition (14) implies that $\mathcal{M}^{(\pm)}(u)$ has a null eigenvector $v^{(\pm)}(u)$,

$$\mathcal{M}^{(\pm)}(u) \ v^{(\pm)}(u) = 0, \tag{20}$$

Note that the matrix $\mathcal{M}^{(\pm)}(u)$ has the symmetry

$$S\mathcal{M}^{(\pm)}(u)S^{-1} = \mathcal{M}^{(\pm)}(u+\eta),$$
 (21)

where

$$S = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}, \qquad S^{p+1} = \mathbb{I}.$$
 (22)

It follows that the null eigenvector $v^{(\pm)}(u)$ satisfies $Sv^{(\pm)}(u) = v^{(\pm)}(u+\eta)$. Thus, its components can be expressed in terms of a function $Q^{(\pm)}(u)$,

$$v^{(\pm)}(u) = (Q^{(\pm)}(u), Q^{(\pm)}(u+\eta), \dots, Q^{(\pm)}(u+p\eta)),$$
(23)

with $Q^{(\pm)}(u+i\pi)=Q^{(\pm)}(u)$. We make the Ansatz

$$Q^{(\pm)}(u) = \prod_{j=1}^{M^{(\pm)}} \operatorname{sh}(u - u_j^{(\pm)}) \operatorname{sh}(u + u_j^{(\pm)} + \eta), \qquad (24)$$

which has the crossing symmetry $Q^{(\pm)}(u) = Q^{(\pm)}(-u - \eta)$. Substituting the expressions for $\mathcal{M}^{(\pm)}(u)$ (15) and $v^{(\pm)}(u)$ (23) into the null eigenvector equation (20) yields the result for the transfer matrix eigenvalues

$$\Lambda^{(\pm)}(u) = h^{(\pm)}(u) \frac{Q^{(\pm)}(u-\eta)}{Q^{(\pm)}(u)} + h^{(\pm)}(-u-\eta) \frac{Q^{(\pm)}(u+\eta)}{Q^{(\pm)}(u)}.$$
 (25)

The asymptotic behavior (13) implies that $M^{(\pm)} = \frac{1}{2}(N-1\pm k)$, where k is the integer appearing in the constraint (4). Analyticity of the eigenvalues (25) implies the Bethe Ansatz equations

$$\frac{h^{(\pm)}(u_j^{(\pm)})}{h^{(\pm)}(-u_j^{(\pm)} - \eta)} = -\frac{Q^{(\pm)}(u_j^{(\pm)} + \eta)}{Q^{(\pm)}(u_j^{(\pm)} - \eta)}, \qquad j = 1, \dots, M^{(\pm)}.$$
 (26)

In short, for case (i), the eigenvalues of the transfer matrix (6) are given by (25), where $h^{(\pm)}(u)$ and $Q^{(\pm)}(u)$ are given by (19), (24) and (26).

In Ref. 17, we have verified numerically that this solution holds also for generic values of η , which is consistent with Refs. 20, 21, 22; and that this solution gives the complete set of 2^N eigenvalues. To illustrate how completeness is achieved, let us consider the case N=4. The integer k in the constraint (4) must therefore be odd, with $-5 \le k \le 5$. The six possibilities are summarized in Table 1.

Table 1.	Completeness	for $N=4$.	For each k ,	there are 2^4	eigenvalues.
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k	# eigenvalues given by $\Lambda^{(+)}(u)$	# eigenvalues given by $\Lambda^{(-)}(u)$
5	16	0
3	15	1
1	11	5
-1	5	11
-3	1	15
-5	0	16

4. Case(ii)

A key feature of case (i) is that the quantity $\Delta(u)$ (5) is a perfect square. We therefore look for additional such cases. For p even, we find that $\Delta(u)$ is also a perfect square if either (a) at most one of the boundary parameters is nonzero; or (b) any two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are arbitrary, the remaining boundary parameters from this set are either η or $i\pi/2$, and $\theta_- = \theta_+$. For definiteness, we focus here on the subcase (b) with α_{\pm} arbitrary, $\beta_{\pm} = \eta$ and N even. Unfortunately, the resulting z(u) (18) is not consistent. To surmount this difficulty, we use a matrix $\mathcal{M}(u)$ which is different from (15), namely 18

$$\mathcal{M}(u) = \begin{pmatrix} \Lambda(u) & -h(u) & 0 & \dots & 0 & -h(-u+p\eta) \\ -h(-u) & \Lambda(u+p\eta) & -h(u+p\eta) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h(u+p^2\eta) & 0 & 0 & \dots & -h(-u-p(p-1)\eta) & \Lambda(u+p^2\eta) \end{pmatrix}$$

where h(u) is $2i\pi$ -periodic. This matrix has the symmetry

$$S\mathcal{M}(u)S^{-1} = \mathcal{M}(u + p\eta), \qquad (28)$$

where S is given by (22). By arguments similar to those used in Sec. 3, we find that the transfer matrix eigenvalues are given by

$$\Lambda(u) = h(u) \frac{Q(u+p\eta)}{Q(u)} + h(-u+p\eta) \frac{Q(u-p\eta)}{Q(u)}, \qquad (29)$$

where h(u) is given by

$$h(u) = 4 \operatorname{sh}^{2N}(u+\eta) \frac{\operatorname{sh}(2u+2\eta)}{\operatorname{sh}(2u+\eta)} \operatorname{ch}^{2}(u-\eta)$$
(30)

$$\times \operatorname{sh}(u-\alpha_{-})\operatorname{sh}(u+\alpha_{+})\frac{\operatorname{ch}\left(\frac{1}{2}(u+\alpha_{-}+\eta)\right)}{\operatorname{ch}\left(\frac{1}{2}(u-\alpha_{-}-\eta)\right)}\frac{\operatorname{ch}\left(\frac{1}{2}(u-\alpha_{+}+\eta)\right)}{\operatorname{ch}\left(\frac{1}{2}(u+\alpha_{+}-\eta)\right)},$$

and Q(u) is given by

$$Q(u) = \prod_{j=1}^{M} \operatorname{sh}\left(\frac{1}{2}(u - u_j)\right) \operatorname{sh}\left(\frac{1}{2}(u + u_j - p\eta)\right), \qquad (31)$$

with M = N + 2p + 1; and the Bethe Ansatz equations are

$$\frac{h(u_j)}{h(-u_j + p\eta)} = -\frac{Q(u_j - p\eta)}{Q(u_j + p\eta)}, \qquad j = 1, \dots, M.$$
 (32)

We have verified numerically the completeness of this solution. The other subcases (a) and (b) are mostly similar. ^a

5. Case(iii)

For p odd, we find that the quantity $\Delta(u)$ (5) is also a perfect square if at most two of the boundary parameters $\{\alpha_-, \alpha_+, \beta_-, \beta_+\}$ are nonzero, and $\theta_- = \theta_+$. For definiteness, we focus here on the case with α_\pm arbitrary, $\beta_\pm = 0$ and N even. As in case (ii), the resulting z(u) (18) is not consistent. To surmount this difficulty, we again use a matrix $\mathcal{M}(u)$ which is different from (15), namely ¹⁹

$$\mathcal{M}(u) = \begin{pmatrix} \Lambda(u) & -\frac{\delta(u)}{h^{(1)}(u)} & 0 & \dots & 0 & -\frac{\delta(u-\eta)}{h^{(2)}(u-\eta)} \\ -h^{(1)}(u) & \Lambda(u+\eta) - h^{(2)}(u+\eta) & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -h^{(2)}(u-\eta) & 0 & 0 & \dots -h^{(1)}(u+(p-1)\eta) & \Lambda(u+p\eta) \end{pmatrix}$$

^aThe exception is the subcase (a) with θ_{\pm} nonzero, for which $Q(u) = \prod_{j=1}^{2M} \operatorname{sh}(u - u_j)$, which is not crossing symmetric. See Sec. 3.3 in Ref. 18.

where $h^{(1)}(u)$ and $h^{(2)}(u)$ are $i\pi$ -periodic. It has the reduced symmetry

$$T\mathcal{M}(u)T^{-1} = \mathcal{M}(u+2\eta), \qquad (34)$$

where $T = S^2$, and S is given by (22). (While (21) implies (34), the converse is not true.) The condition $\det \mathcal{M}(u) = 0$ implies that $\mathcal{M}(u)$ has a null eigenvector v(u),

$$\mathcal{M}(u) \ v(u) = 0 \,, \tag{35}$$

where v(u) satisfies $Tv(u) = v(u+2\eta)$. Thus, its components are expressed in terms of two independent functions $Q_1(u)$, $Q_2(u)$:

$$v(u) = (Q_1(u), Q_2(u), \dots, Q_1(u - 2\eta), Q_2(u - 2\eta)).$$
 (36)

We make the Ansätze

$$Q_{1}(u) = \prod_{j=1}^{M_{1}} \operatorname{sh}(u - u_{j}^{(1)}) \operatorname{sh}(u + u_{j}^{(1)} + \eta),$$

$$Q_{2}(u) = \prod_{j=1}^{M_{2}} \operatorname{sh}(u - u_{j}^{(2)}) \operatorname{sh}(u + u_{j}^{(2)} + 3\eta).$$
(37)

Substituting the expressions for $\mathcal{M}(u)$ (33) and v(u) (36) into the null eigenvector equation (35) yields two expressions for the transfer matrix eigenvalues,

$$\Lambda(u) = \frac{\delta(u)}{h^{(1)}(u)} \frac{Q_2(u)}{Q_1(u)} + \frac{\delta(u-\eta)}{h^{(2)}(u-\eta)} \frac{Q_2(u-2\eta)}{Q_1(u)},
= h^{(1)}(u-\eta) \frac{Q_1(u-\eta)}{Q_2(u-\eta)} + h^{(2)}(u) \frac{Q_1(u+\eta)}{Q_2(u-\eta)}.$$
(38)

Analyticity of these expressions leads to the Bethe Ansatz equations

$$\frac{\delta(u_j^{(1)}) h^{(2)}(u_j^{(1)} - \eta)}{\delta(u_j^{(1)} - \eta) h^{(1)}(u_j^{(1)})} = -\frac{Q_2(u_j^{(1)} - 2\eta)}{Q_2(u_j^{(1)})}, \qquad j = 1, 2, \dots, M_1,
\frac{h^{(1)}(u_j^{(2)})}{h^{(2)}(u_j^{(2)} + \eta)} = -\frac{Q_1(u_j^{(2)} + 2\eta)}{Q_1(u_j^{(2)})}, \qquad j = 1, 2, \dots, M_2. (39)$$

We expect that there are sufficiently many equations to determine all the zeros $\{u_j^{(1)}, u_j^{(2)}\}$ of $Q_1(u), Q_2(u)$, respectively. Functions $h^{(1)}(u)$ (with $h^{(2)}(u) = h^{(1)}(-u-2\eta)$) which ensure the condition $\det \mathcal{M}(u) = 0$ are given by

$$h^{(1)}(u) = 4 \operatorname{sh}^{2N}(u+2\eta), \quad M_2 = \frac{1}{2}N + \frac{1}{2}(3p-1), \quad M_1 = M_2 + 2,$$

 $p = 3, 7, 11, \dots$ (40)

and

$$h^{(1)}(u) = \begin{cases} -2\operatorname{ch}(2u)\operatorname{sh}^{2}u\operatorname{sh}^{2N}(u+2\eta), & M_{1} = M_{2} = \frac{1}{2}N+2p-1, \\ p = 9, 17, 25, \dots \\ 2\operatorname{ch}(2u)\operatorname{sh}^{2}u\operatorname{sh}^{2N}(u+2\eta), & M_{1} = M_{2} = \frac{1}{2}N+\frac{3}{2}(p-1) \\ p = 5, 13, 21, \dots \\ 2\operatorname{ch}(2u)\operatorname{sh}^{2}u\operatorname{sh}^{2N}(u+2\eta), & M_{1} = M_{2} = \frac{1}{2}N+2, \\ p = 1. \end{cases}$$

We have verified numerically the completeness of this solution. Similar results hold for the case with α_-, β_- arbitrary and $\alpha_+ = \beta_+ = 0$, etc.

We observe that this solution represents a generalization of the famous Baxter T-Q relation ⁴, which schematically has the form

$$t(u) Q(u) = Q(u') + Q(u''). (42)$$

Indeed, our result (38) has the structure

$$t(u) Q_1(u) = Q_2(u') + Q_2(u''),$$

$$t(u) Q_2(u) = Q_1(u') + Q_1(u'').$$
(43)

Such generalized T-Q relations, involving two or more independent Q(u)'s, may also appear in other integrable models.

6. Conclusions

We have seen that Bethe Ansatz solutions of the open spin- $\frac{1}{2}$ XXZ quantum spin chain are available for the cases (i)-(iii), for which the quantity $\Delta(u)$ (5) is a perfect square. There may be further special cases for which $\Delta(u)$ is a perfect square, in which case it should not be difficult to find the corresponding Bethe Ansatz solution. Our solution for case (iii) involves more than one Q(u). This is a novel structure, which should be further understood. The general case that $\Delta(u)$ is not a perfect square and/or that $\eta \neq i\pi/(p+1)$ also remains to be understood.

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